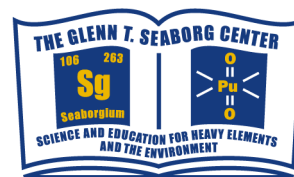




Glenn T. Seaborg Center Seminar



Prof. Luis Seijo
Chemistry Department
Universidad Autónoma de Madrid

How Do Bond Lengths Change upon $f \rightarrow d$ Excitation in Lanthanide and Actinide Hexahalides?

Wednesday, March 3, 2004

4 pm

Building 70A-3377

Abstract

Although it is widely believed that the bond lengths between f-elements and ligands lengthen upon $f \rightarrow d$ excitation, recent quantum chemical ab initio calculations on lanthanide and actinide impurity ions in halide crystals with octahedral coordination show the opposite. Why this is so, and how this depends on the ligand and on the environment of the ML_6 unit is the issue of this seminar.

